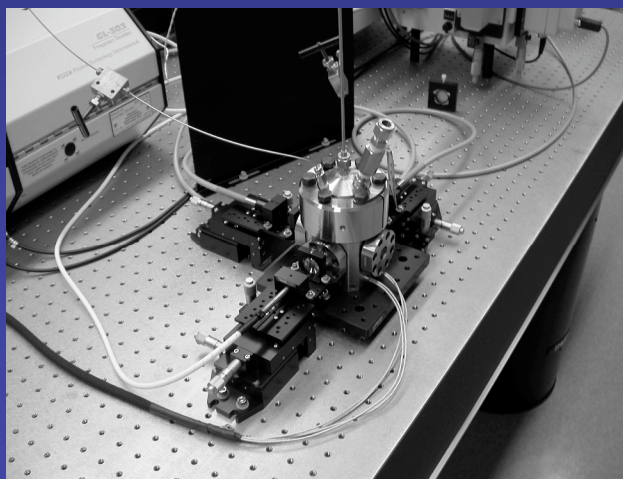


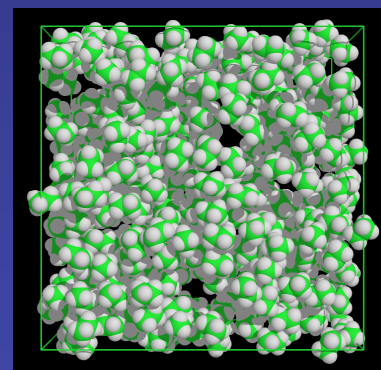
Solvent Effects in Supercritical Fluids

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Despite our understanding of the forces between molecules, we do not yet have an understanding of solvation and solvent effects that has predictive value to the typical experimentalist. We are therefore in the developmental stages of defining how supercritical fluids such as xenon, ethane, carbon dioxide, and trifluoromethane can be used as tools to study solvent effects in photophysical, photochemical, and chemical phenomena. Operation above the critical temperature precludes the complication of phase change when the process of interest is studied as a function of pressure at constant temperature, allowing us to study solvent effects without changing the solvent. Our method includes quantum chemical calculation and molecular dynamics simulation to define the system, and experiment to measure the behavior of the system. Most notably, we used PRF funds and a generous match from the Yeshiva University Office of Academic Affairs to purchase and house major instrumentation, a combined steady-state and time-resolved spectrofluorometer. The time-resolved component of this instrumentation allows us to measure excited state lifetimes as short as 100 picoseconds. Computational progress included determination of the critical temperature of an all-atom ethane model (322.2 K) for the molecular dynamics component of our work. An undergraduate ran simulations to define isotherms close to the critical temperature for a system of 500 ethanes and one pyrazine according to a standard Lennard-Jones potential.



High-pressure stainless-steel vessel mounted on optical table with associated optics for excitation and emission.



Molecular dynamics simulation of all-atom model of 500 ethanes near the critical temperature.